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COMPUTER SIMULATION OF THE
SPUTTERING PROCESS

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COMPUTER SIMULATION OF THE SPUTTERING PROCESS

by

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Lieutenant Commander, United States Navy

Submitted in partial fulfillment of
the requirements for the degree of

MASTER OF SCIENCE
IN
PHYSICS

United States Naval Postgraduate School
Monterey, California

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ABSTRACT

The sputtering of Cu fcc (110), (100) and (111) surfaces by 1- to 10-keV A^+ ions at normal incidence has been investigated by high-speed digital computer techniques. The interatomic repulsions are described by Born-Mayer potentials. The shape of the sputtering ratio curves are in close agreement with the data of Magnuson and Carlston. Ejection patterns in accord with experimental observations are predicted. There is evidence that the sputtering mechanism is not the result of momentum focusing.

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1. Introduction.

The process of ionic erosion of a solid surface is known as sputtering. As pointed out by Cheney, Rogers and Pitkin [1] and Harrison [2], various theoretical models of the sputtering process have been developed since the 1850's when metal from the electrodes in gas discharge tubes was first observed to be transferred to the glass walls of the tubes. In 1923, Kingdon and Langmuir [3] suggested a momentum transfer model, later elaborated upon by Lamar and Compton [4]. This theory was subsequently replaced by a thermal spike model, wherein a local hot spot caused evaporation [5,6]. Later Keywell [7] suggested a model based upon a succession of random collisions, while Harrison [8-13] has proposed several models, including a statistical approach based on neutron diffusion theory, and Monte Carlo techniques. Pease [14] developed a model based upon expressions from radiation damage theory.

However, these early models neglected the ordered arrangement of atoms within the crystal lattice. Current theories are based upon a transfer of energy through collision processes, as developed by Silsbee [15] and Liebfried [16]. In addition to conducting a variety of experiments, Harrison [17,18] combined these energy chain concepts with previous statistical theories into a radiation damage-statistical model [2,19].

Recently, workers in the field of radiation damage have employed digital computers to make theoretical studies. Robinson and Oen [20]

have assumed that the "knock-on" atom interacts through a series of binary (two-body) collisions, while Gibson, Goland, Milgram and Vineyard [21], Erginsoy, Vineyard and Englert [22], and Gay and Harrison [23] have used iteration techniques to numerically integrate the classical equations of motion of a many-body set of atoms.

The present work uses the latter technique to investigate the sputtering of three orientations of a copper crystal subjected to bombardment by an argon ion. This particular combination of elements was chosen for two reasons; first, there is experimental data available for comparison [24,25] and secondly, parameters to be used in the Born-Mayer potentials have been calculated [21,26,27].

Distinction should be made between "sputtering" and "transmission sputtering." As used in this paper, the former pertains to atoms ejected from the bombarded, or front, surface of a solid, while the latter refers to atoms leaving the back surface of a thin crystal. Although the possibility exists that an ejected atom will have one or more electrons stripped away in the sputtering process, this study makes no distinction between neutral atoms and ions.

The sputtering ratio is defined as the number of atoms ejected per incident ion. Several aspects of sputtering have been studied experimentally [24,25,28,29,35], including the sputtering ratio as a function of primary (incoming ion) energy, incidence angle, crystal orientation and target temperature; the angular distribution of ejected atoms, and the energies of these atoms. This study is concerned

quantitatively only with the sputtering ratio as a function of monocrystalline orientation for primary energies in the 1- to 10-keV range and at normal incidence, and qualitatively with a description of the process whereby the crystal atoms are ejected from the lattice, and their angular distribution.

2. The Model

The model employed in this computer simulation program is the result of the combination of many ideas from previous work in the field of radiation damage. An early attempt by Oen, Holmes and Robinson [31] assumed binary collisions but excluded crystal lattice effects. This work suggested that neither the exponentially screened Coulomb potential nor the Bohr hard sphere potential were sufficiently accurate. A later model used by Robinson and Oen [20] placed copper atoms on their proper sites in a face centered cubic lattice. However, this model also considered collisions as binary and assumed that the target atoms did not interact amongst themselves. The Bohr potential and Born-Mayer potential with Gibson 2 parameters [21] were compared. Gibson et. al. [21] also studied effects in the fcc copper crystal, but considered collisions as n-body while comparing several sets of the two parameters of the Born-Mayer potential. Similar work for bcc iron was done by Erginsoy et. al. [22]. More recently, Gay and Harrison [23] employed a somewhat different n-body model. This project uses the Gay-Harrison model but with further modifications, viz:

(1) The stationary immoveable atoms surrounding the crystallite have been removed. The object of this study is the ejection of atoms from the surface, and also, the lattice is stable before bombardment without these stationary atoms.

(2) The crystallite size has been increased to contain the

sputtering event. The (110) sample contains 115 atoms, the (100) has 158, and the (111) contains 150. The (110) sample corresponds to ten planes in the x-direction, five planes in the y-direction, and nine planes in the z-direction. The (100) sample is 7 x 5 x 9, while the (111) is 9 x 5 x 17. The total external dimensions of these three crystallites are approximately the same (see appendix I). As work progressed it was readily determined which atoms were sputtered from the crystallite. Thus, by judicious choice of impact points, the crystallite may be decreased in size to reduce computer running time. This will be done in future studies.

(3) A running report of the motion of every atom versus a final status report has been incorporated.

(4) The impact area for the (111) sample has been chosen to be representative of a "repeat" crystallographic distance rather than just of the first two planes. The repeat distance is the number of layers that must be traversed to repeat the crystal configuration [24]. Thus the projections of the first two layers of the (110) sample, first layer of the (100) sample, and first three layers of the (111) sample are considered. Then symmetry shows that the rectangle for the (110), and triangles for the (100) and (111) orientations, will completely describe the crystallites if repeated (see figs. 1-3). Thirty-six impact points were assigned to the (110) representative rectangle, while 21 points were assigned to the (100) and (111) triangles (see fig. 4).

(5) There is no "target atom" as defined by Gay and Harrison, but the impact points are all near a "central" atom of the crystal-lite front surface.

(6) The "time step multiplier" is 0.10 for all impact points except those in which a "head-on" collision with a front surface lattice atom occurs. In the latter case, a value of 0.05 was found to be necessary to minimize total energy error.

In addition to n-body collisions, major ideas used by Gay and Harrison and retained in this program include the double iteration technique, lack of thermalizing motion, concepts of representative areas and time step intervals mentioned previously, the "lattice unit," disregard of interactions between the primary and lattice electrons (although provision is made for inclusion in future studies), use of Gibson 2 parameters in the Born-Mayer potential for copper-copper interactions, and omission of cohesive effects and restoring forces. The last point is justified by time considerations; the sputtering event is complete in a relatively short period, one-tenth to one-hundreth of the time necessary for these effects to commence [23].

Harrison, Carlston and Magnuson [26] state that the repulsive exponential Born-Mayer potential function of the form $V(r) = \exp(A+Br)$, where B is always negative, appears to be adequate for most high energy collision dynamics in a lattice. Initially, the program was run using the Gibson 2 parameters in the Born-Mayer potential for

both the argon-copper and copper-copper interactions. These parameters are not valid for the argon-copper system. The use of these constants resulted in a sputtering ratio versus primary energy curve of improper shape; the curve decreased with increasing energy with no sign of the experimental [24] maximum around 3- to 5-keV. Subsequently, an argon-copper potential was employed for the argon-copper interactions, while the Gibson 2 was retained for the copper-copper system. This A-Cu potential is also of the Born-Mayer form and uses semi-empirical parameters calculated by Harrison et. al. [26] from experimental data collected by Magnuson and Carlston [33]. The sputtering ratio curve obtained with this two potential approach exhibited a peak in the proper region, but the sputtering ratio magnitude was too low at high energies. To increase this ratio the A-Cu potential was "hardened" by increasing "A" in the $V(r)$ expression from the calculated value of 11.435 to 12.25. Figures 5,6 and 7 result when the tabulated parameters are used in the Born-Mayer potential function:

System	A	B (lattice unit) ⁻¹
A-Cu	12.25	-7.597
Cu-Cu	10.024	-9.197

The computer program is a mixture of Fortran 60 and Fortran Symbolic language (see appendix II). The runs were conducted on a Control Data Corporation 1604 computer. Running time for each impact

point was five minutes for the (110) sample, nine minutes for the (111) and from ten to 15 minutes for the (100). Very generally, the program constructs the lattice, bombards the crystallite with a single primary, performs the iteration procedure to determine forces and displacements at the proper time steps, and stops when the total potential energy of all the atoms is less than 0.5 eV, or at a time step chosen by experience so that events of interest have already occurred. The output consists of the position and velocity of each atom with a total energy greater than thermal, assumed to be 0.25 eV (see appendix IV). Output is received when the run is 25%, 50%, 75% and 100% complete.

At the end of the runs the totals of kinetic plus potential energies differed from the primary initial energies (the lattice has no energy until disturbed) by an average of 1%. This error is considered well within the uncertainties inherent in the model, especially the kinematic simplifications of the iteration procedure.

3. Results

A. GENERAL DESCRIPTION OF THE SPUTTERING PROCESS

When energy from the primary is transferred to lattice atoms through the n-body collision process, these atoms (secondaries) are displaced from their sites. The secondaries also interact in a series of collisions, and eventually some will gain momentum back towards the crystal surface. If any atoms have energies great enough to overcome the surface binding energy they will emerge from the crystal. Very generally, this is the sputtering process.

Cheney et. al. [1] have stated that sputtering is expected to be great when there is a large transfer of energy from the primary to the crystal lattice occurring reasonably near the surface, a rapid reversal of the momentum vector of the primary, a mechanism for the transfer of energy back to the surface, an easy escape of surface atoms and a comparatively large atomic volume or mass. Relatively open crystal structures permitting deep penetration of the primary results in a low sputtering yield. Thus, the yield is dependent upon the orientation of the crystal [24]. However, a crystal which has a history of radiation damage may not permit channeling [20,32] in open crystallographic directions, in which case the sputtering yield may actually increase. Other works [25,30] have suggested that the ejection of atoms along preferred directions is the result of momentum focusing chains. In light of this research some of these concepts must be modified.

B. THE INDIVIDUAL ORIENTATIONS

1. The (110) Sample

Inspection of figure 8 reveals that most of the ejected atoms come from the region near the impact rectangle. A detailed analysis of the mechanism whereby a few of these atoms are sputtered will lead to an understanding of the sputtering process. In the following discussion "low" energy refers to 1 keV and "high" energy refers to 10 keV primary energy.

Atom 14 is ejected most often. At low energy the impact points which cause sputtering of this atom are those in the upper right quarter of the representative rectangle. At high energy the impact points in the center of the rectangle cause it to sputter. The number of impact points which result in ejection is essentially independent of the primary energy.

For all cases in which this atom is sputtered, it is driven towards the crystal interior by interaction with the primary. "Down" and "left" motion is also imparted. The atom is repulsed by atoms lying in the second plane, no. 33 usually, and is reflected towards the front surface. This process imparts momentum to no. 33 towards the back of the crystal, which accounts for the relatively few times that it is sputtered. At 10 keV no. 14 gains enough momentum to interact also with atom no. 8 after rebounding from no. 33.

Atom 15 is a major contributor to the 3 keV peak of the sputtering ratio curve. Impact points that cause this atom to sputter lie

in the right center portion of the representative rectangle at low energy, and the bottom center at high energy. No. 15 is ejected less often with increasing primary energy. Channeling, resulting in deeper ion penetration before interaction, occurs with greater primary energy, which explains this behavior. The mechanism which ejects 15 is dependent upon interaction at the front surface. The atom is initially directed to the right by the primary. The ensuing collision with no. 16 rebounds no. 15 out of the crystal. Additionally, at higher energies, the primary rebounds from no. 14 and ejects 15 directly by getting behind it before interacting strongly. Primaries entering at impact points in the left half of the rectangle do not interact strongly enough with no. 15 to impart the velocities necessary to collide with no. 16.

Atom 37 is also a contributor to the sputtering ratio peak. The impact points responsible are in the upper left quarter of the rectangle, where the primary "bypasses" no. 14 and interacts mainly with second layer atoms, nos. 38 and 39 in particular. No. 38 is driven in and to the left in a direction to be behind no. 37 before approaching closely enough to interact. Thus 37 acquires motion out of the crystal and towards the left.

Comparable to atom no. 15, the impact points that sputter no. 37 lie in a region where the primary is channeled at higher energies, with resultant less ion-atom interaction at the crystal front planes. No. 37, then, is also sputtered less at higher ion energies.

At low energy atom 19 is initially given a velocity up, in and towards the left. Interactions with no. 24 at the front surface and no. 43 in the second plane result in reflection towards the front. The impact region responsible for sputtering no. 19 is also the upper left quarter, with a few points around the perimeter of this area. With increased primary energy impact points where channeling occurs cease to cause sputtering of this atom, but the points outside of this area still eject no. 19. At high energy the primary is reflected from the third layer atoms 59 and 64, and takes no. 19 with it as it comes back out the front.

At 10 keV atoms 13, 38 and 40, in addition to nos. 14 and 15, are sputtered often. Atom 13 is sputtered as a result of the primary driving 14 behind 13, whence the latter acquires motion out and to the left, rebounding from no. 12 before emerging. Atom 38 is sputtered by an identical mechanism, except that the primary, after interacting with no. 39 gets behind no. 38, and the latter interacts with 37 before it comes out of the crystal. In an analogous manner no. 39 sputters atom 40.

An interesting, but not surprising, phenomenon is the number of atoms sputtered from deep (third or greater) layers as a function of primary energy. There are none sputtered at 1 keV, one at 3 keV, four at 5 keV, and six at 10 keV. This behavior would be expected since the primary penetrates further with increased energy and transfers momentum to the deeper atoms.

As mentioned previously in section 2, the two potential approach resulted in a sputtering ratio curve of the proper shape. To adjust this curve to the ordinates obtained experimentally [24], a "threshold energy" notion is employed. An arbitrary value is chosen, and the assumption made that any atom with kinetic energy less than this amount (in the direction normal to the surface) will not escape the crystal. A family of curves result (see fig. 5) from which an estimate can be made of the binding energy of atoms to a crystal surface. Thus 4 eV is the value estimated for the copper (110) surface since this figure yields a curve with the best fit to experimental data.

An analysis of the angular distribution of the sputtered atoms leads to some extremely interesting results. At 1 keV primary energy one third of the ejected atoms leave the surface with equal velocities in the "x" and "z" directions. These velocities range from one-half to equal the "y" velocity. That is, a large percentage of atoms emerge approximately in the $\langle 111 \rangle$ direction, but nearer to the surface normal. One-sixth of the atoms emerge in the $\langle 110 \rangle$ direction while the remainder are randomly oriented. Thus the model predicts a deposit spot pattern consisting of a central spot, four $\langle 111 \rangle$ spots and considerable haze.

At 10 keV one-third of the atoms emerge in the $\langle 110 \rangle$ direction, one-fifth in approximately the $\langle 111 \rangle$ direction, and one-fifth near the $\langle 100 \rangle$ direction. At this energy the model predicts the central

spot, four $\langle 111 \rangle$ spots, plus two $\langle 100 \rangle$ spots which may merge with the central spot, and less haze than obtained at 1 keV.

2. The (111) Sample

As an example of the sputtering mechanism, consider atom 19, which is ejected most often. This atom has motion imparted by the primary "up" and towards the right (see fig. 3). The collision with atom 25 alters its momentum vector towards the front surface.

The sputtering ratio curve is shown in figure 7. Although the shape of the curve approaches the experimental data for 6 eV threshold energy, the magnitudes disagree significantly. Inspection of the figure shows that different threshold energies do not yield a family of curves, but that the curve shape is altered with changes in energy.

The deposit pattern for this orientation consists of a central spot with three large surrounding spots corresponding to the $\langle 011 \rangle$ directions.

3. The (100) Sample

Analysis of the paths of sputtered atoms reveals that the ejection mechanism is consistent with the other two orientations. Figure 9 shows that the atoms near the impact area are ejected most often.

The sputtering ratio curve is shown in figure 6. There is close agreement with the experimental data [24] in the 1-5 keV range. At 10 keV the sputtering ratio is too high, indicating that the potential function may be too hard at higher energies.

The deposit pattern for this orientation consists of a heavy concentration of atoms in the center, with lesser concentrations in diagonally opposite quadrants.

4. Discussion

A. The (110) Surface

As mentioned in section 3, the majority of the atoms which are sputtered come from the region around the impact area. This observation indicates a model which accounts for sputtering as the result of the direct transfer of momentum from the primary ion to the lattice atoms, rather than by chaining. The mechanism whereby crystal atoms are ejected supports this view. Although there are differences in this mechanism at high and low energies, there is no evidence in this study that momentum focusing plays a role in the sputtering process.

The threshold energy necessary to achieve agreement with the experimental sputtering ratio curve is considered to be quite reasonable. The value of 4 eV is typical of the heat of sublimation, which is less than the energy required to displace an atom from its lattice site. The displacement energies which have been determined are applicable to interior atoms, while surface atoms are expected to be less tightly bound.

The model successfully predicts the shape of the sputtering ratio curve. Discrepancies between experimental and theoretical magnitudes can be attributed to the approximations of the potential function in the theory or the modification of the crystal during irradiation experiments.

The deposit spot pattern observed by Nelson, Thompson, Farmery

and Hall [37] is also successfully predicted. Although the experimental group was working at higher energies, deposit patterns above 10 keV are expected to have the same general features. At 1 keV this study predicts a spot pattern similar to those obtained by Southern et al. [25]. This group worked with a $\langle 011 \rangle$ sample but crystallographic considerations show that the $\langle 110 \rangle$ should have similar patterns. The model agrees qualitatively with the experimental results of the latter group in two important respects; (1) the non-central ejection spots are closer to the surface normal than would be expected by consideration of crystal geometry, and (2) the neighboring rows influence the motion of the ejected atoms.

B. The (111) Surface

The sputtering mechanism is similar to the (110) sample in that momentum focusing is not evident. The atoms are ejected as the result of sequences of first and second layer collisions.

The estimated binding energy is taken to be 6 eV, the value which yields the proper shape of the sputtering ratio curve. Discrepancies in magnitude between the model and experiment are considered to be the result of failure of the potential function parameters. "Hardening" the potential for future studies of this orientation may give better agreement.

Selection of different binding energies have the greatest effect on the magnitude of the sputtering ratio at lower energies. This indicates that lower primary energies result in ejection of lower

energy atoms.

The deposit pattern experimentally observed by Southern et. al. [25] is successfully predicted.

C. The (100) Surface

Results of bombardment of this surface also indicate that momentum focusing is not evident. Sputtering is the result of first or second layer collisions.

The estimated binding energy is 2.6 eV. Additional investigation in the 5-10 keV range is being conducted to bring the sputtering ratio curve into closer agreement with experimental observations. The shape of the curve is sensitive to the threshold energy, which has the greatest effect on magnitude at 3 keV (see fig. 6). The possibility exists, in nature, that the binding energy of the crystal is a function of the amount of disturbance, and hence a function of primary energy.

The deposit pattern corresponds to "half" of the pattern observed by Southern et al. [25]. That is, there is a central spot and two $\langle 011 \rangle$ spots. Bombarding the crystallite in a mirror image impact triangle may yield the other two $\langle 011 \rangle$ spots.

5. Conclusions

This computer simulation program is considered adequate in most respects. The model predicts the proper shape of the sputtering ratio curves, the angular distribution of ejected atoms, binding energies in the neighborhood of expected values, and magnitudes of the sputtering ratio for two of the three orientations.

Momentum focusing does not enter into the sputtering mechanism for the argon-copper system in the 1- to 10-keV range. However, there are cases of chain transmission of momentum of surface atoms parallel to the surface.

There is a wealth of experimental data available which requires theoretical exploration. Further work using this model should include study of the energy distribution of ejected atoms, sputtering ratio as a function of primary incoming direction, inclusion of thermalized motion of lattice atoms, and investigation of transmission sputtering, all for additional systems of elements and other energy ranges. The computer program should be expanded to include a graph plot output of the sputtering ratio curve and a plot of the angular and energy distributions of the ejected atoms.

The computer programming assistance of LT Peter D. Stogis is gratefully acknowledged. I am indebted to Prof. Don E. Harrison Jr. for his guidance and assistance in all phases of the work.

Note in support of argument. Recent work on argon sputtered

lithium by Stein, Malakhof and Smith [38] led the authors to suggest that, at low energy, there is small likelihood of extensive penetration of the lattice by the primary. Hence, there is little chance for a large number of n-body collisions yielding a focused momentum change to take place. The lobes of the distribution pattern of the sputtered atoms are believed to be created by a limited number of n-body collisions near the surface. (This effect should be even more pronounced for copper since the mass of the target atoms is considerably greater than lithium).

FACE CENTERED CUBIC (110)

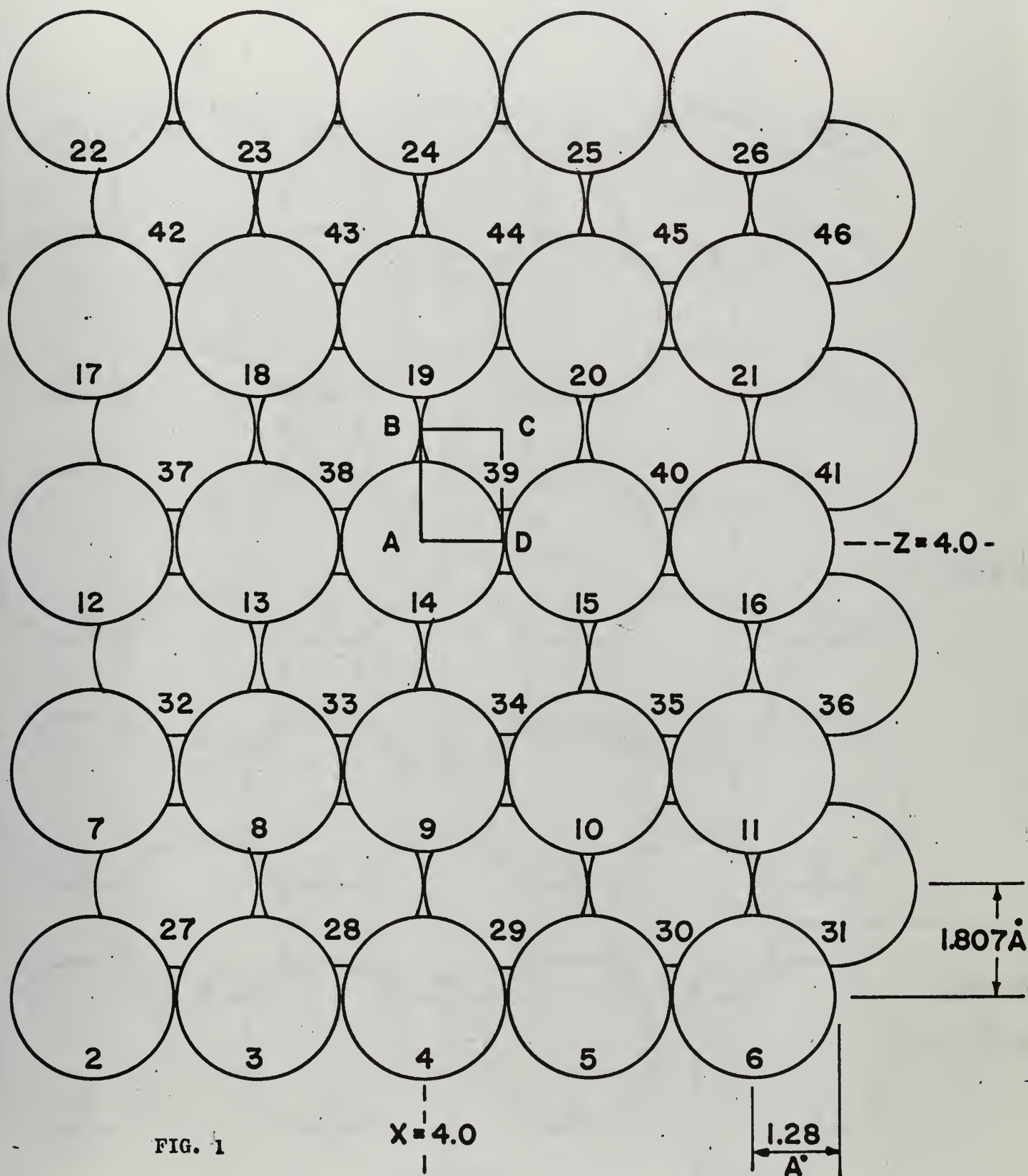


FIG. 1

FACE CENTERED CUBIC (100)

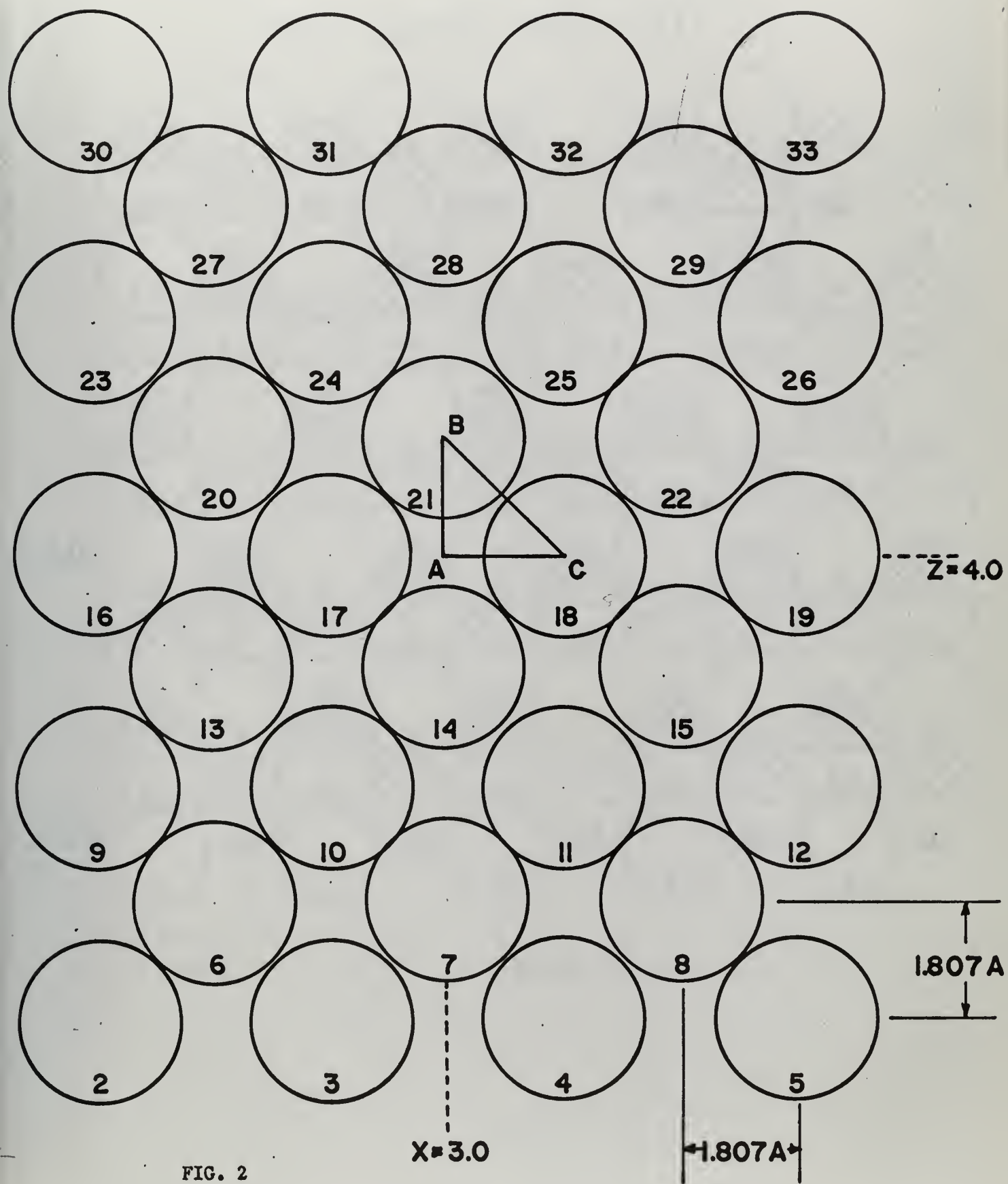


FIG. 2

Face Centered Cubic (111)

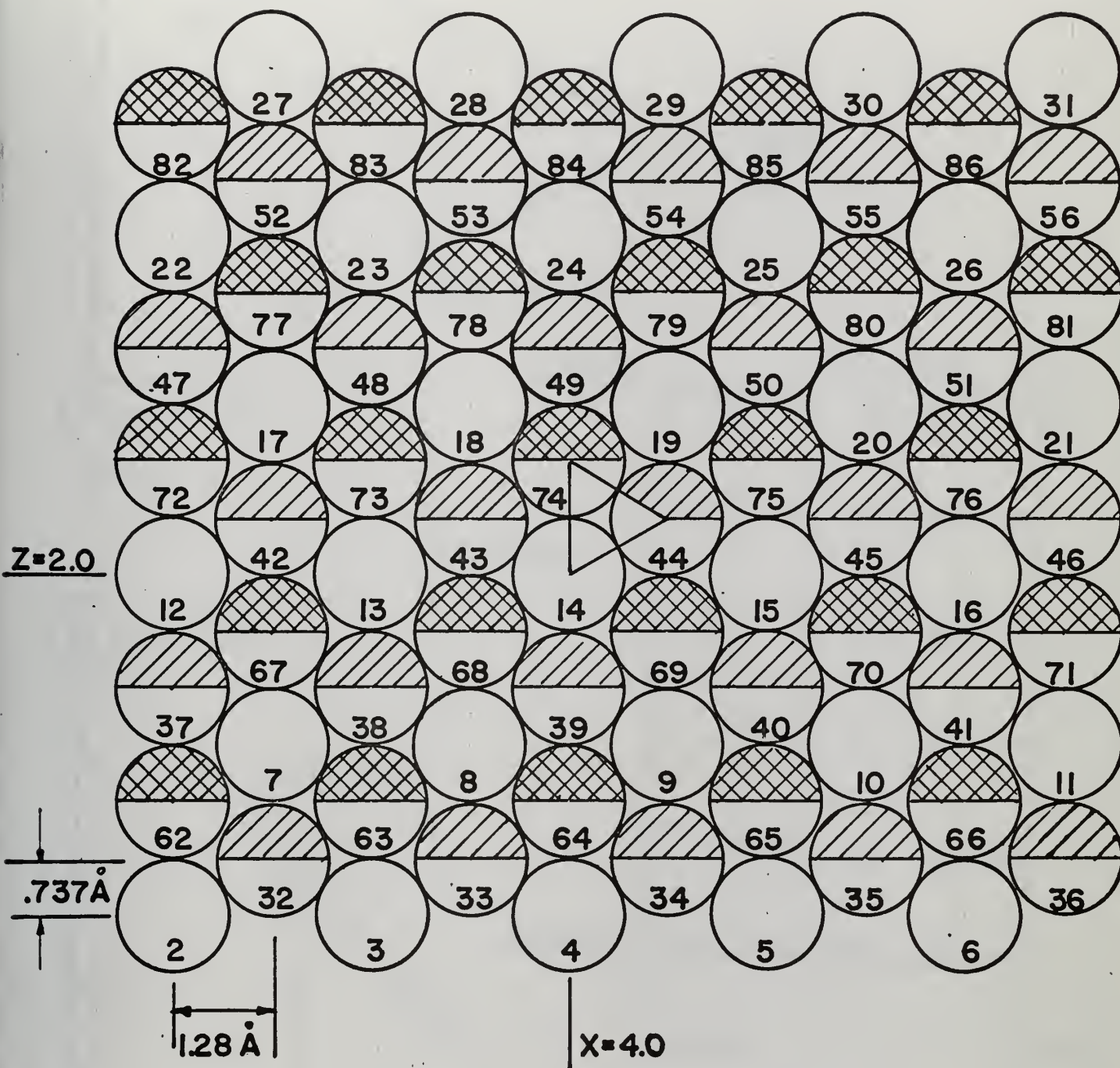


FIG. 3

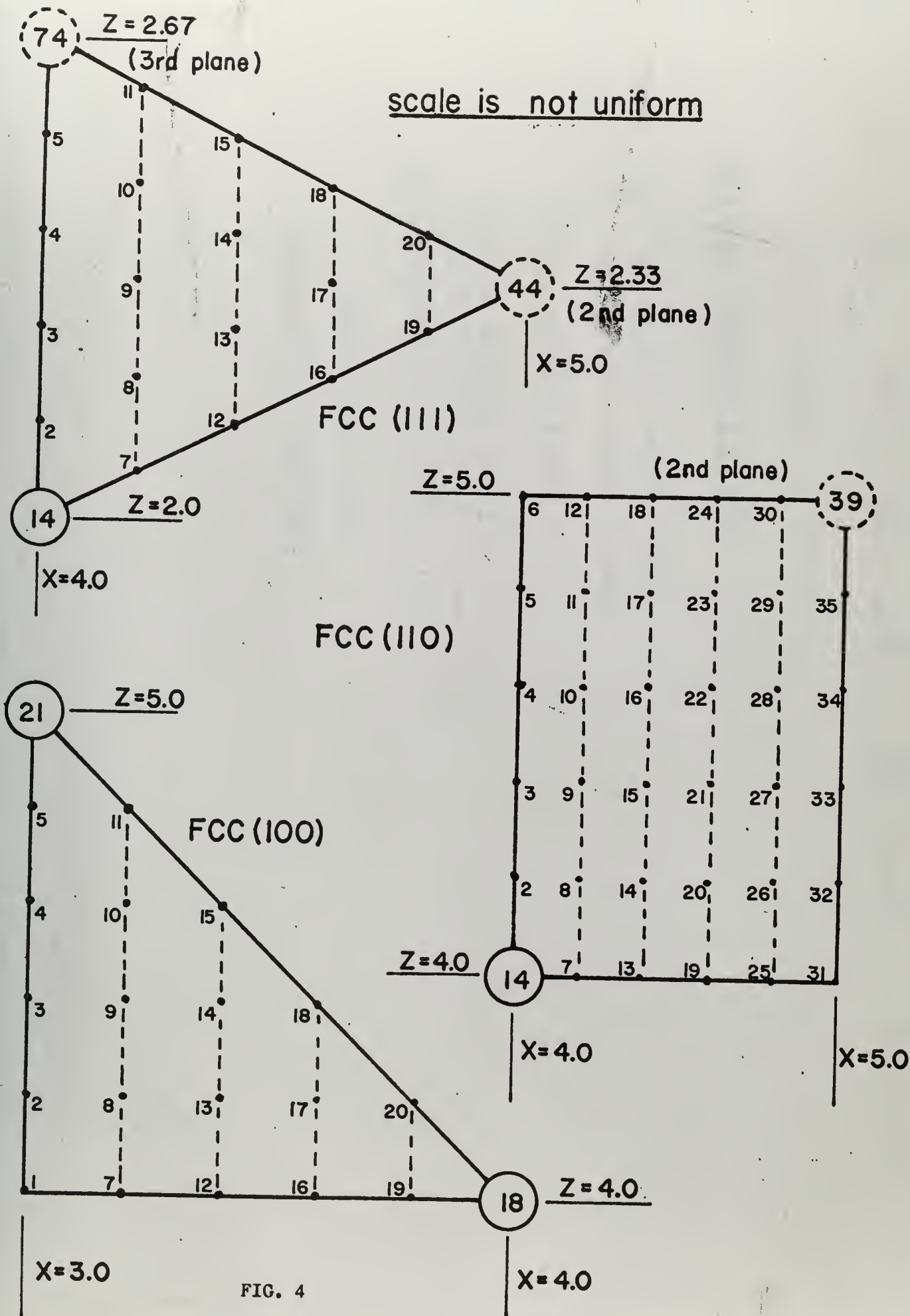


FIG. 4

ARGON - COPPER (110) Orientation

⊙ Magnuson-Carlston Data
— 4 eV binding energy
- - - 5 eV binding energy

Two Potential Model

argon - copper A = 12.25, B = - 7.60

copper - copper A = 10.02, B = - 9.20

SPUTTERING RATIO

FIG. 5

Primary Energy (keV)

10

9

8

7

6

5

4

3

2

1

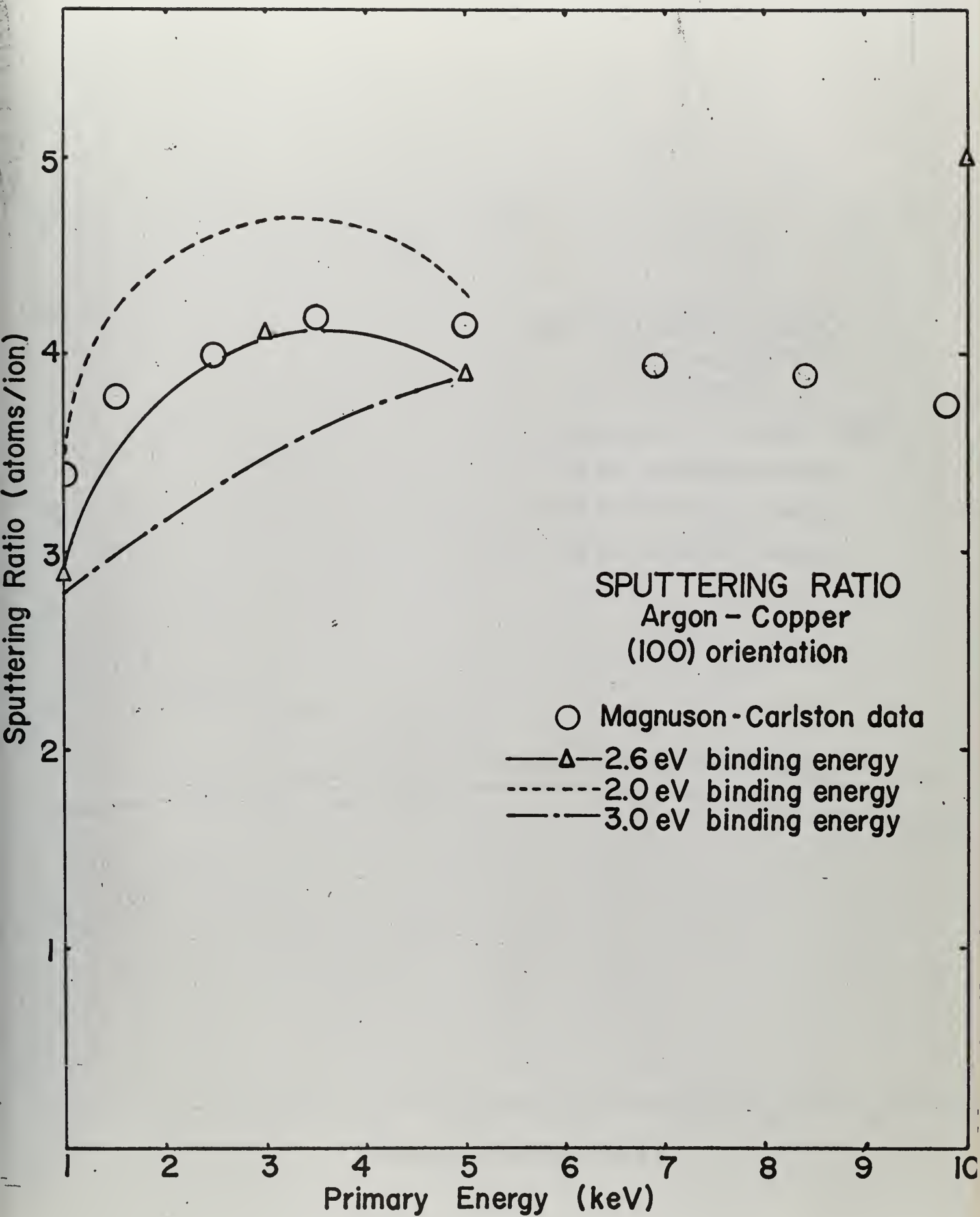


FIG. 6

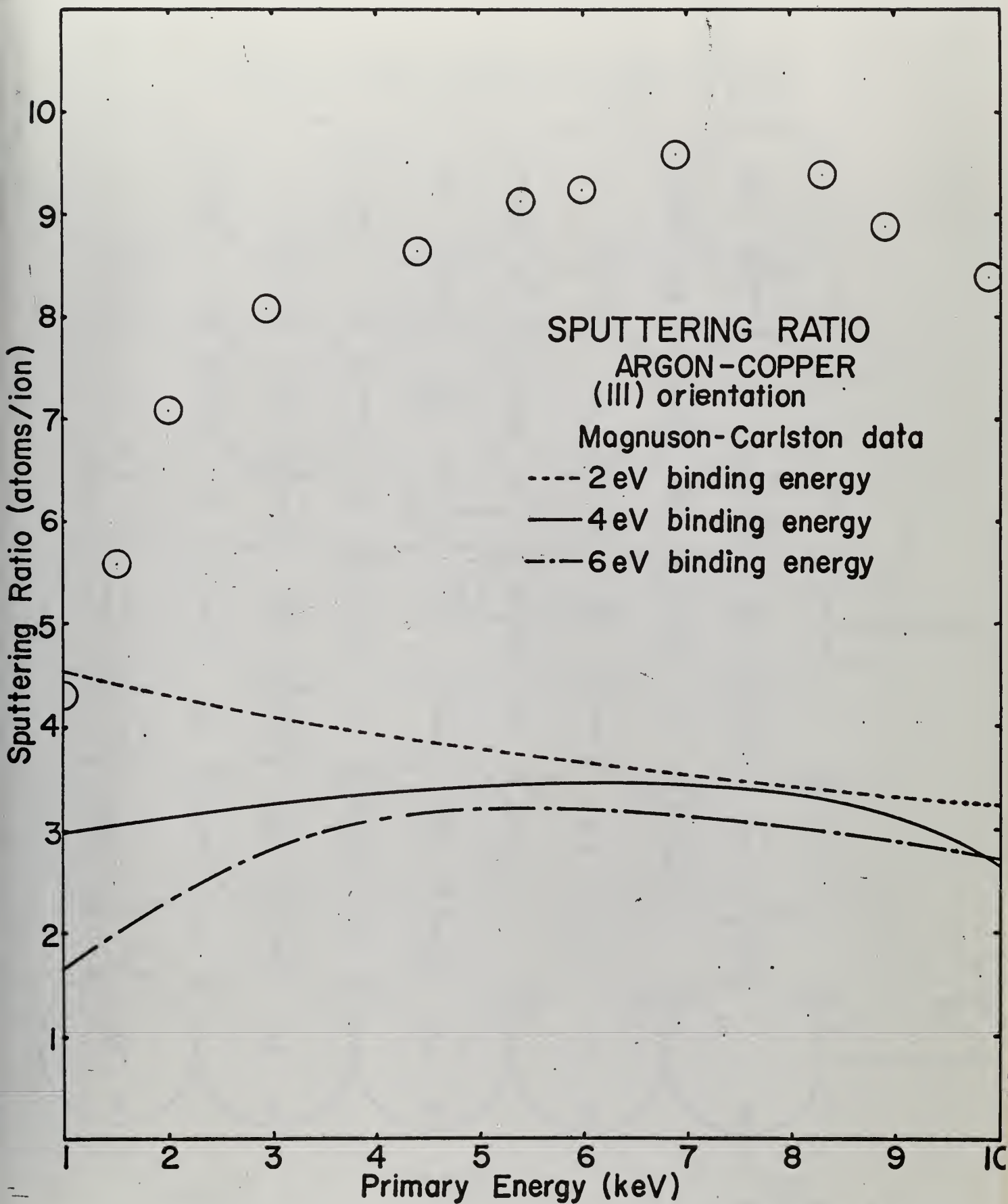


FIG. 7

FACE CENTERED CUBIC (110)

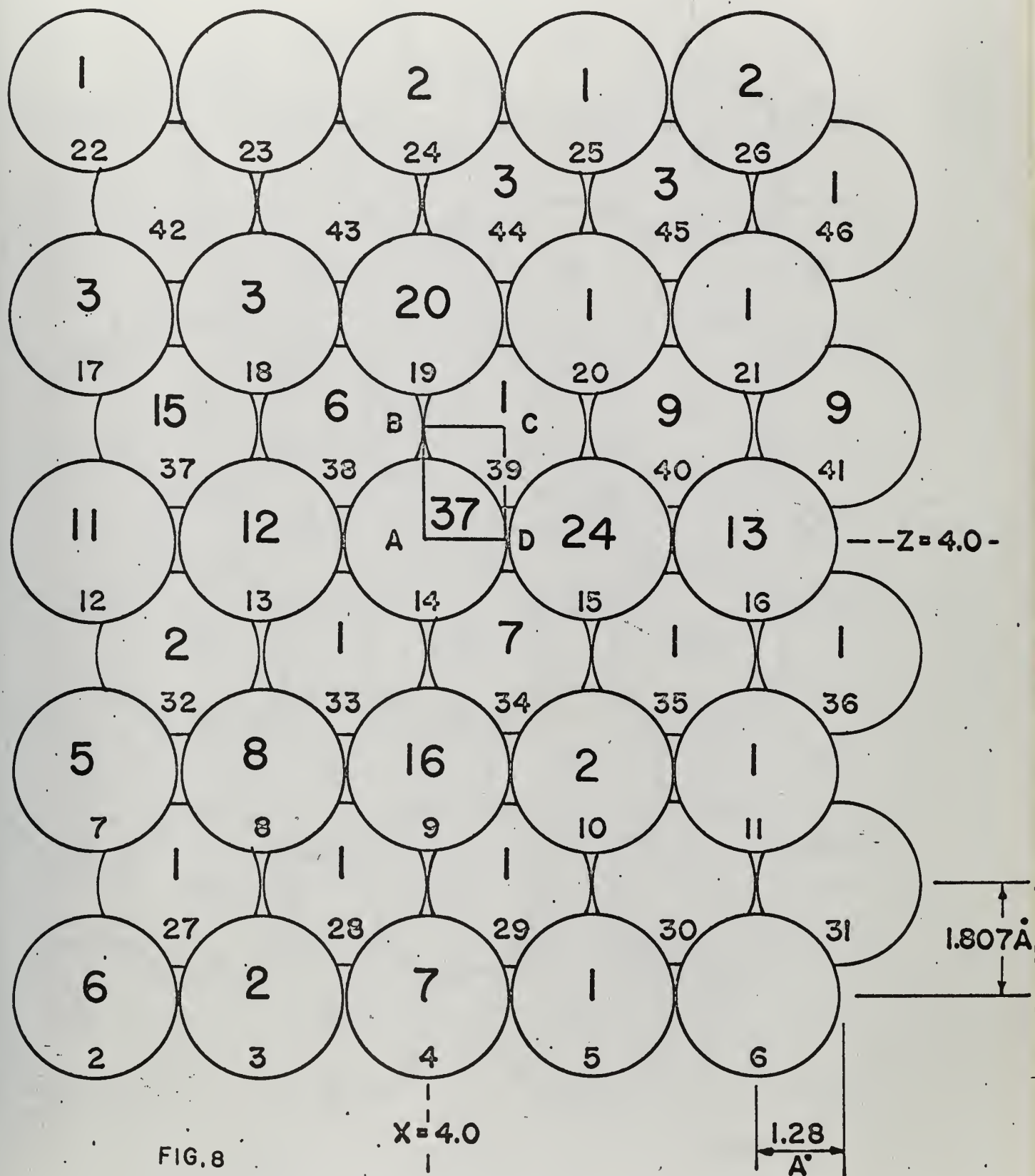


FIG. 8

FACE CENTERED CUBIC (100)

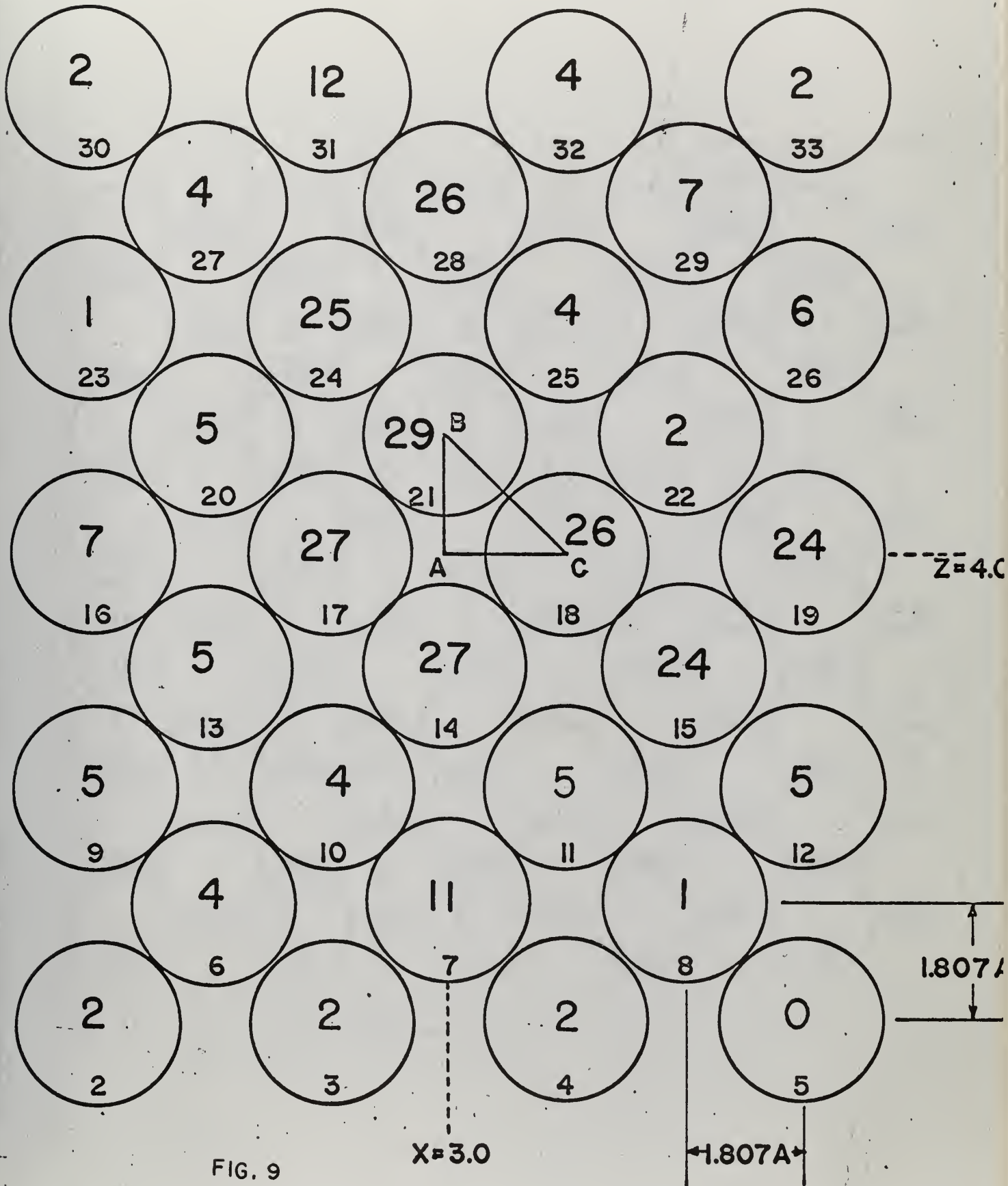


FIG. 9

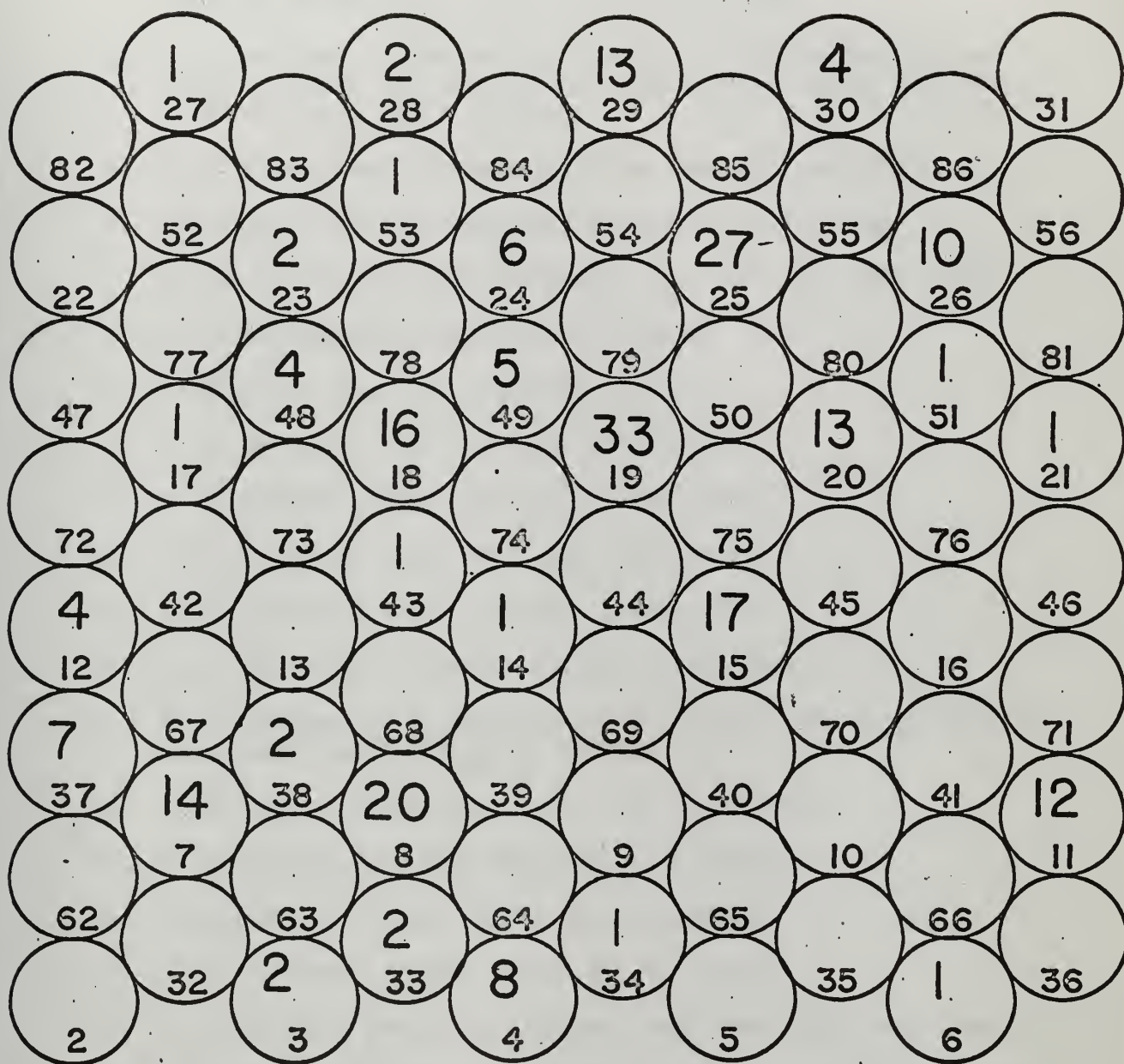


FIG. 10

6. BIBLIOGRAPHY

1. K. B. Cheney, E. E. Rogers and E. T. Pitkin, Research on Experimental Evaluation of Sputtering Yield Rates. Aerospace Research Laboratories Report ARL 63-125 (1963).
2. D. E. Harrison, A Theoretical Model of the Sputtering Process. Transactions of the 8th National Symposium on Vacuum Technology. Pergamon Press, 1962: 259-264
3. K. H. Kingdon and I. Langmuir, Phys. Rev. 22, 148 (1923).
4. E. S. Lamar and K. T. Compton, Science 80, 541 (1934).
5. A. von Hippel and E. Blechschmidt, Ann. Phys. 86, 1006 (1928).
6. C. H. Townes, Phys. Rev. 65, 319 (1944).
7. F. Keywell, Phys. Rev. 97, 1611 (1955).
8. D. E. Harrison, Phys. Rev. 93, A652 (1954).
9. D. E. Harrison, Phys. Rev. 100, A1234 (1955).
10. D. E. Harrison, Phys. Rev. 102, 1473 (1956).
11. D. E. Harrison, Phys. Rev. 105, 1202 (1957).
12. D. E. Harrison, J. Chem. Phys. 32, 1336 (1960).
13. D. T. Goldman, D. E. Harrison and R. Coveyou, Oak Ridge National Laboratory Report ORNL-2729 (1959).
14. R. S. Pease, Rendiconti S.I.F. 13, 158 (1960).
15. R. H. Silsbee, J. Appl. Phys. 28, 1246 (1957).
16. G. Liebfried, J. Appl. Phys. 31, 117 (1960).
17. D. E. Harrison, J. Appl. Phys. 32, 924 (1961).
18. D. E. Harrison and G. D. Magnuson, Phys. Rev. 122, 1421 (1961).
19. D. E. Harrison, Energy Chain Effects in the Sputtering Process. Le bombardment ionique, theories et applications, France. Centre National de la Recherche Scientifique. Colloques internationaux 113, 173 (1962).

20. M. T. Robinson and O. S. Oen, Phys. Rev. 132, 2385 (1963) and earlier papers.
21. J. B. Gibson, A. N. Goland, M. Milgram and G. H. Vineyard, Phys. Rev. 120, 1229 (1960).
22. C. Erginsoy, G. H. Vineyard and A. Englert, Phys. Rev. 133, A595 (1964).
23. W. L. Gay and D. E. Harrison, Phys. Rev. 135, A1780 (1964).
24. G. D. Magnuson and C. E. Carlston, J. Appl. Phys. 34, 3267 (1963).
25. A. L. Southern, W. R. Willis and M. T. Robinson, J. Appl. Phys. 34, 153 (1963).
26. D. E. Harrison, C. E. Carlston and G. D. Magnuson, On the Kinetic Emission of Electrons from Monocrystalline Targets (to be published).
27. J. A. Brinkman, USAEC Report NAA-SR-6642 (1962).
28. See, for example, papers by V.I. Veksler, G. K. Wehner, R. S. Nelson or M. W. Thompson, in addition to reference (1).
29. D. E. Harrison and O. C. Yonts, Survey of High Energy Sputtering Experiments. American Rocket Society Symposium (1961).
30. R. S. Nelson and B. W. Farmery, Phil. Mag. 8, 693 (1963); R.S. Nelson, J. Nuc. Matl. 10, 154 (1963); M. W. Thompson, Phys. Lett. 6, 24 (1963); J. B. Sanders and J. M. Fluit, Physica 30, 129 (1964).
31. O. S. Oen, D. K. Holmes and M. T. Robinson, J. Appl. Phys. 34, 302 (1963).
32. J. A. Davies, G. C. Bell, F. Brown and B. Domeij, Can. J. Phys. 42, 1070 (1964); R. S. Nelson and M. W. Thompson, Phil. Mag. 8, 1677 (1963); G. R. Piercy, M. McCargo, F. Brown and J. A. Davies, Can. J. Phys. 42, 1116 (1964); J. Beeler and D. Besco, Phys. Rev. 134, A530 (1964).
33. G. D. Magnuson and C. E. Carlston, Phys. Rev. 129, 2409 (1963).
34. R. W. Leeds, Computer Simulation Studies of Copper Atoms in (110) Channels of Copper Crystals. Thesis, U.S. Naval Postgraduate School (unpublished).
35. J. M. Fluit, C. Snoek and J. Kistemaker, Physica 30, 144 (1964).

36. G. K. Wehner, G. S. Anderson and H. Laegreid, General Mills Mechanical Division Report 1930 (1960).
37. R. S. Nelson, M. W. Thompson, B. W. Farmery and M. J. Hall, Phys. Lett. 2, 124 (1962).
38. R. P. Stein, V. Malakhof and H. P. Smith Jr., J. Appl. Phys. 36, 1504 (1965).

APPENDIX I

CRYSTAL GEOMETRY

A. Lattice Dimensions

Orientation	Dimensions (L.U.)		
	X	Y	Z
(110)	$9 \times .707 = 6.36$	$4 \times .707 = 2.83$	$8 \times 1.0 = 8.0$
(100)	$6 \times 1.0 = 6.0$	$4 \times 1.0 = 4.0$	$8 \times 1.0 = 8.0$
(111)	$9 \times .707 = 6.36$	$4 \times 1.155 = 4.62$	$5.67 \times 1.22 = 6.94$

$$1 \text{ L.U.} = 1.807 \text{ \AA}$$

B. Atomic Numbering System

Orientation	Y-plane number				
	1	2	3	4	5
(110)	2-26	27-46	47-71	72-91	92-116
(100)	2-33	34-64	65-96	97-127	128-159
(111)	2-31	32-61	62-91	91-121	122-151

APPENDIX II PROGRAM LISTING

SECTION 1

```

PROGRAM TWOPT
  POTF(X)=EXPFF(EXA+EXB*X)
  FORC(X)=EXPFF(FXA+EXB*X)
  PPOTF(X)=EXPFF(PEXA+PEXB*X)
  PFORCF(X)=EXPFF(PFXA+PEXB*X)
  DIMENSION RX(1000),RY(1000),RZ(1000),FX(1000),FY(1000),FZ(500)
  DIMENSION LCUT(500)
  DIMENSION VX(1000),VY(1000),VZ(500)
  DIMENSION PKEY(500)
  DIMENSION PPE(1000),PKE(1000),PTE(1000)
  DIMENSION RXK(1000),RYK(1000),RZK(1000)
  DIMENSION RXI(1000),RYI(1000),RZI(1000)
  DIMENSION IH(5)
  COMMON RXK,RYK,RZK,RXI,RYI,RZI
  LOC(ILIM=57B,INOW=50B)
  FORMAT(1H)
  FORMAT(1H1)
  FORMAT(80H)

1000
1001
1010
1011
1012
1014
1015
1016
1017
1020
1030
1040
1050
1060
1070
1080
1090
1091
1092
1093
  /)
  FORMAT(4F10.5,5A8)
  FORMAT(/,29H BULLET INCOMING LOCATION X= F6.3, 5H Z= F6.3,
110H ENERGY= F10.1,24H TIME STEP MULTIPLIER= F5.3, /)
  FORMAT(5H EXA=,F9.5,6H EXB=,F9.5,6H FXA=,F9.5,16H LATTICE UNIT
1=,F5.3,15H ANGSTROM UNITS,5X,17H BINDING ENERGY=,F5.1,3H EV,/)
  FORMAT(36X,6H PEXA=,F9.5,6H PEXB=,F9.5,6H PFXA=,F9.5,/)
  FORMAT(40X,5A8,/)
  FORMAT(2F10.5)
  FORMAT(118,3F10.5,3E10.2,4F10.4)
  FORMAT(107H
1VZ
1040
1050
1060
1070
1080
1090
1091
1092
1093
  ATOM DX DY TE KE(Y) VX VY
  KE
  PE
  DZ
  KE(Y)
  VX
  VY
  FORMAT(2F8.3,3F5.2,E8.2,3F8.5,I5,2I3,I2,A4)
  FORMAT(36X,14H BULLET MASS=,F7.3,15H TARGET MASS=,F7.3,10X,16HP
  POSITION NUMBER,A4,/)
  FORMAT(22H ELAPSED TIME (SEC)=,E10.4,19H THERMAL CUTOFF=,F5.3
1,3H EV,22H ENERGY LOSS CONSTANT=,IPE10.3,OP,11H TIMESTEP=,I6,/)
  FORMAT(1X,F10.3,24H EV,TOTAL KINETIC ENERGY,,F10.3,27H EV,TOTAL PD
1POTENTIAL ENERGY,F10.3,17H EV,TOTAL ENERGY)
  FORMAT(36X,14H COSINE TO X=,F7.5,16H, COSINE TO Y=,F7.5,/)
  FORMAT(29H TARGET POINT ON CRYSTAL X=,F6.3,5H Z=,F6.3,28H C
1UTOFF ENERGY THRESHOLD=,F6.1,15H SAMPLE SIZE (,I3,2H X,I3,2H X,
2I3,2H ),/)
  FORMAT(315,2E20.11,3F8.2,/)
  FORMAT(14,3F12.8,3E16.9,2F10.4,I2)
  FORMAT(105X,4HPAGE,I3,/,1H1)

```


SECTION 2

4 READ INPUT TAPE 2, 9040, GMAS, TMAS, BX, BY, BZ, EV, DTI, COX, COY, NTT, NS, NDO

SECTION 3

```

IX=10
IY=5
IZ=9
IXP=(IX+1)/2
IYP=(IY+1)/2
IZP=(IZ+1)/2
RD=1.0/SQRTF(2.0)
SCX=RD
SCY=RD
SCZ=1.0
M=2
JT=0
DO 60 J=1,IY
KT=0
DO 59 K=1,IZ
IT=0
DO 58 I=1,IX
ENQ(0)LDA(IT)LRS(1)QJP2(16)LDA(JT)LRS(1)QJP2(57)LDA(KT)LRS(1)
QJP2(57)SLJ(20)
16 LDA(JT)LRS(1)QJP3(57)LDA(KT)LRS(1)QJP3(57)
20 X=IT
RX(M)=X*SCX
X=JT
RY(M)=X*SCY
RZ(M)=KT
M=M+1
IT=IT+1
57 CONTINUE
58 KT=KT+1
59 CONTINUE
60 JT=JT+1
CONTINUE
LL=M-1
DO 63 I=2,LL
VX(I)=0.0
VY(I)=0.0
VZ(I)=0.0
63 CONTINUE

```


SECTION 4

```

VOL=SQRTF(EV/HGMAS)
VX(1)=VOL*COX
VY(1)=VOL*COY
TIME=BY/VY(1)
COZ=1.0-COX*COX-COY*COY
COZ=ABSF(COZ)
COZ=SQRTF(COZ)
VZ(1)=VOL*COZ
RX(1)=SCX*8X+TIME*VX(1)
RY(1)=BY
RZ(1)=SCZ*BZ+TIME*VZ(1)
DO 66 I=1,LL
LCUT(I)=0
RXI(I)=RX(I)
RYI(I)=RY(I)
RZI(I)=RZ(I)
DT=DTI*CVD/VOL
DXS=0.0
DYS=0.0
DZS=0.0
TIME=0.0
NT=0
NL=0
NLDTI=1.0/DTI
ENI5(C)ENI6(O)
NPAGE=1
DTOD=CT/CVD
HDTOM=0.5*DT/PTMAS
QDTOM=0.5*HDTOM
HDTOMB=0.5*DT/PGMAS
QDTOMB=0.5*HDTOMB

```

66

68

SECTION 5

```

70 DO 75 I=1,LL
75 LDA(ZE)STA1(FX)STA1(FY)STA1(FZ)
105 LDA(ZE)STA1(IPOT)STA1(IPKE)STA1(SPE)
110 LDA(LL)SAU(L+2)ENI1(0)ENI(0)
110 ISK1(*)SLJ(L+2)SLJ(200)ENI(0)
    LDA1(LCUT)AJP1(110)
    LDA(LL)SAU(L+3)
    ENA1(0)SAL(IP1)LIL2(IP1)ENI(0)
120 ISK2(*)SLJ(L+2)SLJ(110)ENI(0)
    LDA2(LCUT)AJP1(120)
    DRX = RX(J) - RX(I)
    +SSK(DRX),SLJ(L+2),+SCM(MASK),+FSB(ROE),AJP2(120).
    DRY=RY(J)-RY(I)
    +SSK(DRY),SLJ(L+2),+SCM(MASK),+FSB(ROE),AJP2(120).
    DRZ=RZ(J)-RZ(I)
    +SSK(DRZ),SLJ(L+2),+SCM(MASK),+FSB(ROE),AJP2(120).
150 LDA(DRX)FMU(DRX)STA(DIST)LDA(DRY)FMU(DRY)FAD(DIST)STA(DIST)LDA(DRZ)
155 FMU(DRZ)FAD(DIST)STA(DIST)FSB(ROE2)AJP2(120)
    DIST = SQRTF(DIST)
    ENA1(0)INA(-1)AJP1(156)ENI(0)
    FORCE=PFORCF(DIST)-PFCR
    GO TO 157
156 FORCE=FORCE(DIST)-FRC
157 LDA(FORCE)FSB(FM)AJP3(120)
    FJD = FORCE / DIST
    FA = DRX * FOD
    FB = DRY * FOD
    FC = DRZ * FOD
160 FX(J) = FX(J) + FA
    FY(J) = FY(J) + FFB
    FZ(J) = FZ(J) + FFC
165 FX(I) = FX(I) - FFA
    FY(I) = FY(I) - FFB
    FZ(I) = FZ(I) - FFC
    SLJ(120)
200 CONTINUE

```


SECTION 6

```

211 LDA(LL)SAU(L+2)ENI1(1)ENI(0)
   ISK1(*)SLJ(L+2)SLJ(220)ENI(0)
   LDA1(RY)AJP3(214)
   SLJ(211)
214 FAD(SCY)AJP3(211)AJP(211)
   LDA1(FY)FAD(BIND)STA1(FY)
   SLJ(211)
220 LDA(INDEX)AJP1(260)
   INDEX=1
   I=1
   RXK(I)=RX(I)
   RYK(I)=RY(I)
   RZK(I)=RZ(I)
   RX(I)=(VX(I))+FX(I)*HDTOMB)*DTOD+RX(I)
   RY(I)=(VY(I))+FY(I)*HDTOMB)*DTOD+RY(I)
   RZ(I)=(VZ(I))+FZ(I)*HDTOMB)*DTOD+RZ(I)
   DO 250 I=2,LL
   RXK(I)=RX(I)
   RYK(I)=RY(I)
   RZK(I)=RZ(I)
   RX(I)=(VX(I))+FX(I)*HDTOMB)*DTOD+RX(I)
   RY(I)=(VY(I))+FY(I)*HDTOMB)*DTOD+RY(I)
   RZ(I)=(VZ(I))+FZ(I)*HDTOMB)*DTOD+RZ(I)
250 CONTINUE
   GO TO 105

```

SECTION 7

```

260 INDEX=0
   TIME=TIME+DT
   NT=NT+1
   NL=NL+1
   I=1
   RX(I)=RXK(I)+(VX(I))+FX(I)*QDTOMB)*DTOD
   RY(I)=RYK(I)+(VY(I))+FY(I)*QDTOMB)*DTOD
   RZ(I)=RZK(I)+(VZ(I))+FZ(I)*QDTOMB)*DTOD
   VX(I)=VX(I)+FX(I)*HDTOMB
   VY(I)=VY(I)+FY(I)*HDTOMB
   VZ(I)=VZ(I)+FZ(I)*HDTOMB
   LDA(ZE)STA1(FX)STA1(FY)STA1(FZ)
   DO 300 I=2,LL
   RX(I)=RXK(I)+(VX(I))+FX(I)*QDTOMB)*DTOD
   RY(I)=RYK(I)+(VY(I))+FY(I)*QDTOMB)*DTOD
   RZ(I)=RZK(I)+(VZ(I))+FZ(I)*QDTOMB)*DTOD
   VX(I)=VX(I)+FX(I)*HDTOMB
   VY(I)=VY(I)+FY(I)*HDTOMB
   VZ(I)=VZ(I)+FZ(I)*HDTOMB
   LDA(ZE)STA1(FX)STA1(FY)STA1(FZ)
300 CONTINUE

```


SECTION 8

```

310 LDA(ILIM)SUB(INOW)INA(-10)STA(ISHUT)AJP3(950)
    LDA(NS)SUB(NT)AJP(400)AJP3(400)
    LDA(NL)SUB(NLDTI)AJP(410)AJP3(70)
400 CONTINUE
    WRITE(OUTPUT)TAPE 3,9010
    WRITE(OUTPUT)TAPE 3,9016,IH
    WRITE(OUTPUT)TAPE 3,9050,GMAS,TMAS,PNUM
    WRITE(OUTPUT)TAPE 3,9080,COX,COY
    WRITE(OUTPUT)TAPE 3,9012,RXI(1),RZI(1),EV,DTI
    WRITE(OUTPUT)TAPE 3,9090,BX,BZ,EI,IXP,IYP,IZP
    WRITE(OUTPUT)TAPE 3,9014,EXA,EXB,FXA,CVR,BENERGY
    WRITE(OUTPUT)TAPE 3,9015,PEXA,PEXB,PEXA
    WRITE(OUTPUT)TAPE 3,9060,TIME,THERM,CELS,NT
    WRITE(OUTPUT)TAPE 3,9030

```

SECTION 9

```

410 DO 500 I=1,LLPE)STA1(PTE)STA1(PKE)
500 LDA(ZE)STA1(PTE)STA1(PKE)
    LDA(LL)SAU(L+2)ENI(1(0)ENI(0)
510 ISK1(*)SLJ(L+2)SLJ(600)ENI(0)
    LDA1(LCUT)AJP1(510)
    LDA(LL)SAU(L+3)
520 ENA1(0)SAL(IP1)LIL2(IP1)ENI(0)
    ISK2(*)SLJ(L+2)SLJ(510)ENI(0)
540 LDA2(LCUT)AJP1(520)
    DRX=RX(J)-RX(I)
    +SSK(DRX),SLJ(L+2),+SCM(MASK),+FSB(ROE),AJP2(520).
    DRY=RY(J)-RY(I)
    +SSK(DRY),SLJ(L+2),+SCM(MASK),+FSB(ROE),AJP2(520).
    DRZ=RZ(J)-RZ(I)
    +SSK(DRZ),SLJ(L+2),+SCM(MASK),+FSB(ROE),AJP2(520).
    LDA(DRX)FMU(DRX)STA(DIST)STA(DIST)FAD(DIST)STA(DIST)LDA(DRZ
1)FMU(DRZ)FAD(DIST)STA(DIST)FSB(ROE2)AJP2(520)
556 DIST = SQRTF(DIST)
    ENA1(0)INA(-1)AJP1(560)ENI(0)
    POT=PPOTF(DIST)-PPIC
    GO TO 565
560 POT=POTF(DIST)-PIC
565 PPE(I)=PPE(I)+0.5*POT
    PPE(J)=PPE(J)+0.5*POT
    TPOT = TPOT + POT
    SLJ(520)
600 CONTINUE

```


SECTION 10

```

ENI1(1)ENI(0)
I=1
PKE(1)=HGMAS*(VX(1)*VX(1)+VY(1)*VY(1)+VZ(1)*VZ(1))
FAD(TPKE),STA(TPKE),LDA1(PKE),FAD1(PPE),STA1(PTE).
PKEY(1)=HGMAS*(VY(1)*VY(1))
BRY=0.0
LDA(LL)SAU(L+2)ENI1(1)ENI(0)
ISK1(*)SLJ(L+2)SLJ(660)ENI(0)
PKE(1)=HTMAS*(VX(1)*VX(1)+VY(1)*VY(1)+VZ(1)*VZ(1))
FAD(TPKE),STA(TPKE),LDA1(PKE),FAD1(PPE),STA1(PTE).
PKEY(1)=HTMAS*(VY(1)*VY(1))
LDA1(RY)AJP3(630)
SLJ(610)
610 FAD(SCY)AJP3(640)AJP(640)
LDA1(RY)FAD(BRY)STA(BRY)
SLJ(610)
620 LDA(BRY)FAD(SCY)STA(BRY)
SLJ(610)
630
640

```

SECTION 11

```

660 LDA(NS)SUB(NT)AJP(700)AJP2(753)
700 DO 750 I=1,LL
LDA1(PTE),FSB(THERM),AJP3(750).
DX=RX(I)-RX(I)+DXS
DY=RY(I)-RY(I)+DYS
DZ=RZ(I)-RZ(I)+DZS
WRITE OUTPUT TAPE 3,9020, I,DX,DY,DZ,VX(I),VY(I),VZ(I),PKE(I),PPE(
1),PTE(I),PKEY(I)
750 CONTINUE
BF=BRY*BIND
TE=TPOT+TPKE+BF
WRITE OUTPUT TAPE 3,9000
WRITE OUTPUT TAPE 3,9070,TPKE,TPOT,TE
WRITE OUTPUT TAPE 3,9093,NPAGE

```


SECTION 12

```

753 NPAGE=NPAGE+1
    NS=NS+ND
    LDA(NT)SUB(NTT)AJP2(950)
    EMAX=0.0
    DO 760 I=1,LL
    LDA1(PKE)FSB(FM)AJP3(760)LDA1(PPE)FSB(FM)AJP3(757)
    LDA(EMAX)FSB1(PKE)AJP2(760)LDA1(PKE)STA(EMAX)SIL1(ISS)SLJ(760)
757 LCUT(I)=1
760 CONTINUE
    LDA(TPOT)FSB(QUIT)AJP3(950)
    LDA(ISS)INA(-1)AJP(770)SLJ(780)
770 VOL=SQRTF(PKE(1)/HGMAS)
    GO TO 790
780 VOL=SQRTF(PKE(ISS)/HTMAS)
790 DT=DTI*CVD/VOL
    LDA(DT)FSB(SLOW)AJP2(950)
    NL=0
    GO TO 68

```

SECTION 13

```

950 CONTINUE
    WRITE OUTPUT TAPE 3,9090,BX,BZ,EI,IXP,IYP,IZP
    WRITE OUTPUT TAPE 3,9012,RXI(1),RZI(1),EV,DTI
    WRITE OUTPUT TAPE 3,9091,NT,NS,NPAGE,TIME,DT,DXS,DYS,DZS
    WRITE OUTPUT TAPE 3,9092,(I,RX(I),RY(I),RZ(I),VX(I),VY(I),VZ(I),PK
1E(I),PPE(I),LCUT(I),I=1,LL)
    WRITE OUTPUT TAPE 3,9093,NPAGE
    LDA(ISHUT)AJP3(9999)
    IF(SENSE SWITCH 2) 9999,4
9999 STOP
    END
    END

```


APPENDIX III

PROGRAM DISCUSSION

A. Brief Explanation of the Program.

The descriptions below pertain to the sections of the program as outlined in appendix II.

Section 1: Allocates space in computer cells for arrays of various properties of the atoms; establishes input and output formats; establishes the Born-Mayer form for both potentials.

Section 2: Defines various constants and variables; reads input data.

Section 3: Constructs the crystallite.

Section 4: Commences the bombardment by assigning the primary its proper direction and velocity.

Section 5: Force double iteration procedure. This section calculates the forces on the atoms by use of a triangular matrix, then later recalculates the forces after the atoms have been displaced by the original forces. The average of these forces is then applied to the initial positions of the atoms to determine their displacements.

Section 6: Determines the tentative positions of the atoms under the forces calculated in section 5, then returns the program to section 5 for force recalculation.

- Section 7: Establishes positions of the atoms under the average force. Calculates velocities of all atoms.
- Section 8: Tests the current time step to see if output is called for. If affirmative, prints output headings.
- Section 9: Calculates atomic separations from the positions determined in section 7. Calculates potential energies based upon these separations and the Born-Mayer parameters.
- Section 10: Computes kinetic energies of the atoms from their velocities. Calculates the total binding energy of escaping atoms.
- Section 11: If the time step is such that output is called for this section prints displacement, velocity, kinetic and potential energies of each atom with a total energy greater than 0.25 eV.
- Section 12: Indexes any atoms which have escaped from the crystal so that they will be excluded from future "do" loops (an attempt to reduce computer running time). Recalculates the time step interval on the basis of the most energetic atom still in the crystal. Tests the total potential energy and time step interval against values selected to be indicative of the end of a run. Continues the run if tests are negative.
- Section 13: Prints the status report at the end of the run, which includes the position, velocity, kinetic and potential energies of each atom. Returns the program to the input step for reception of the next impact point data.

B. Terms not defined in Leeds' Program [34].

PPOTF(X), PFORCF(X), PFXA, PFRC and PPTC are the argon-copper functions which correspond to the copper-copper functions POTF(X), FORCF(X), FXA, FRC and PTC.

LCUT indexes any atoms which have been ejected from the crystal as explained under section 12, appendix II A.

NLDTI is the number of time steps between recalculation of DT, the time step interval.

NL is an index used to test if NLDTI time steps have elapsed since DT was last recalculated.

QUIT is the value of total potential energy chosen to test for program shutdown.

SLOW is the value of the time step interval chosen to test for program shutdown.

BENERGY is the binding force assigned to the crystal surface, in eV.

CVB is the conversion factor to make BENERGY consistent with units employed within the program.

BRY is the cumulative distance from the front surface of all atoms that have been ejected.

BF is the cumulative binding energy of these ejected atoms. The value is determined by a force x distance calculation ($BENERGY \times CVB \times BRY$).

ARGON-COPPER(100) SPUTTERING

GIBSON 2 COPPER-COPPER

POSITION NUMBER L100

BULLET MASS= 39.940 TARGET MASS= 63.540

COSINE TO X = .00000, COSINE TO Y =1.00000

BULLET INCOMING LOCATION X= 3.200 Z= 4.600 ENERGY= 5000.0 TIME STEP MULTIPLIER= .100

TARGET POINT ON CRYSTAL X= 3.200 Z= 4.600 CUTOFF ENERGY THRESHOLD = 25.0 SAMPLE SIZE (4 X 3 X 5)

EXA= 10.02407 EXB= -9.19667 FXA= -8.60230 LATTICE UNIT =1.807 ANGSTROM UNITS BINDING ENERGY = .0 EV

PEXA= 12.25000 PEXB= -7.59700 PFXA= -6.56745

ELAPSED TIME (SEC) = .1933E-13 THERMAL CUTOFF = .250 EV ENERGY LOSS CONSTANT= .000E-01 TIMESTEP = 75

ATOM	DX	DY	DZ	VX	VY	VZ	KE	PE	TE	KE(Y)
1	94409	37348	59107	69E+04	15E+05	83E+04	72.8979	.0000	72.8979	48.6121
10	-.06567	.06303	-.06172	-.21E+03	-.26E+02	-.20E+03	5.1036	.9140	6.0333	2.2983
11	-.00527	-.00049	-.00340	-.31E+03	-.36E+02	-.17E+03	.0417	.5615	.6034	.0004
12	-.00591	-.00162	-.00291	-.31E+03	-.36E+02	-.19E+03	.0404	.5149	.5554	.0034
14	-.00294	-.00129	-.00373	-.31E+03	-.36E+02	-.12E+04	112.0934	.8190	112.9128	58.1565
15	-.00294	-.00129	-.00373	-.31E+03	-.36E+02	-.12E+04	16.7604	.4.9674	21.7270	73.3333
18	3.89446	1.15210	1.37980	-.81E+03	-.10E+04	-.70E+05	636.5710	.0000	636.5710	73.2979
19	3.19868	1.21636	1.31682	-.34E+04	-.39E+04	-.57E+04	19.5867	.6247	20.2111	5.0153
21	-.1.20716	3.55826	2.32688	1.12E+04	1.17E+05	1.8E+04	105.8092	.8257	174.6349	41.9319
23	-.02298	-.00100	-.00155	-.12E+03	-.17E+03	-.69E+04	116.7632	.7399	117.5031	100.5269
36	1.00008	-.00100	-.00082	-.12E+03	-.17E+03	-.85E+02	5.0625	.4335	10.2509	.0040
43	1.45012	-.19590	-.10266	-.37E+03	-.37E+03	-.12E+05	52.7426	.4.4884	53.2242	1.6961
46	1.00052	-.02766	-.02208	-.38E+03	-.37E+03	-.14E+05	484.9774	.1408	485.2072	4.6507
49	-.00257	-.02257	-.00043	-.55E+02	-.69E+05	1.0E+05	17.8895	.2295	25.0158	286.0389
54	-.00036	-.00274	-.00239	-.35E+03	-.30E+03	-.44E+04	17.8895	.7.1353	25.0158	.0293
56	-.00036	-.00274	-.00239	-.35E+03	-.30E+03	-.44E+04	56.6102	.1.4611	58.3503	.0287
59	-.00255	-.04132	-.00170	-.10E+02	-.35E+03	1.2E+05	1.1050	.3.2426	5.0866	6.3155
60	-.02105	-.01801	-.03915	-.85E+03	1.1E+04	1.1E+04	1.1717	.2296	5.0866	.3781
62	-.01444	-.00558	-.00489	-.30E+03	1.2E+03	1.0E+03	.0360	.2296	5.0866	.0045
63	-.00178	-.00269	-.00094	-.30E+03	1.2E+03	1.0E+03	.0089	.2296	5.0866	.0005
67	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
68	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
71	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
74	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
75	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
76	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
79	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
80	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
86	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
88	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
90	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
103	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
111	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
112	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
121	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
125	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
131	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
143	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
147	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
147	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005
156	-.00135	-.00023	-.00054	-.30E+03	1.2E+03	1.0E+03	.0022	.2296	5.0866	.0005

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